

Science in the Age of AI: Is Your Research Ready for the Digital Revolution?



Leibniz ScienceCampus
**Digital Transformation
of Research**

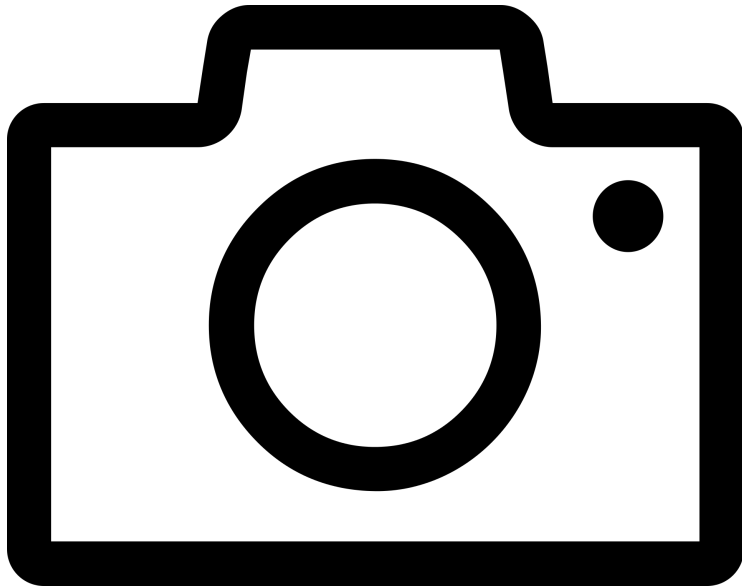
Sonja Schimmmler

Harald Sack, Anna Jacyszyn, Felix Bach



Interdisciplinary Colloquium on Digitalisation of Research, FIZ Karlsruhe, 17 July 2025

Photos and recording



Pixabay, ste_phania



www.youtube.com/@DiTraRe

Agenda

Science in the Age of AI: Is Your Research Ready for the Digital Revolution?



Sonja Schimmler
Fraunhofer FOKUS, Technische
Universität Berlin



Anna Jacyszyn
FIZ Karlsruhe - Leibniz Institute
for Information Infrastructure



Harald Sack
FIZ Karlsruhe - Leibniz Institute
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KIT AIFB



Felix Bach
FIZ Karlsruhe - Leibniz Institute
for Information Infrastructure

1. Welcome and introduction
2. DiTraRe - who are we?
3. Is Your Research Ready for the Digital Revolution?
4. Data Infrastructures as a Foundation for AI Projects
5. Discussion session
6. Lunch @ Casino

Interdisciplinary Colloquium on Digitalisation of Research

We want to use the colloquium as a **regular** possibility to highlight and **discuss** the manifold aspects of digitalisation of research with experts and interested scientists.



- Monthly event: **every first Thursday at 11:00** (~~10:30~~) with rare exceptions
- **Hybrid** format
- **Different on-site locations** to foster interdisciplinary exchange

www.ditrare.de/en/ditrare-colloquium

Schedule

www.ditrare.de/en/ditrare-colloquium

Slot available 2 October.

07.08.2025 11:00–12:00	TBA (AI in Biomedical Engineering)	Till Keller , Department of Cardiology and Angiology, Medical Center, University of Freiburg, Bad Krozingen + Justus Liebig University Giessen, Giessen
04.09.2025 11:00–12:00	TBA (PUNCH4NFDI LLM-based chatbot for creating workflows for physicists and astronomers)	Arman Khalatyan , Leibniz Institute for Astrophysics Potsdam (AIP)
02.10.2025 11:00–12:00	Slot available	Slot available , suggest your speaker in discussion forum (top of the webpage) or ditrare@fiz-karlsruhe.de
06.11.2025 11:30–12:30	Machine Learning in Professional Soccer <u>Abstract</u>	Daniel Memmert , German Sport University Cologne, Institute of Exercise Training and Sport Informatics; Katja Keller , Karlsruhe Institute of Technology, Institute of Sports and Sports Science (KIT IfSS); Claudia Niessner , Karlsruhe Institute of Technology, Institute of Sports and Sports Science (KIT IfSS)
04.12.2025 11:00–12:00	TBA	Stefan Dietze , GESIS Leibniz Institute for the Social Sciences + Heinrich Heine University Düsseldorf




Discussion forum

Continue discussions after
the event:

- Introduce yourself
- Meet others
- Exchange ideas
- Collaborate
- Discuss the talk
- Suggest speakers
- ...



www.ditrare.de/en

-  General discussion
-  The last colloquium
-  Upcoming events

Newsletter

www.ditrare.de/en/newsletter

Forum

www.ditrare.de/en/forum

Leibniz ScienceCampus *Digital Transformation of Research* (DiTraRe)

DiTraRe

Leibniz ScienceCampus *Digital Transformation of Research*

- Growth core to **establish new research branch.**



+



- Planned as a **4+4 years** project (start: September 2023).
- Funded by the Leibniz Association + FIZ KA + KIT.
- Analyse the process of **digitalisation of research.**
- **Multilevel interdisciplinary approach.** → We start with 4 specific use cases.

DiTraRe Use Cases



1

Sensitive Data
in Sports
Science

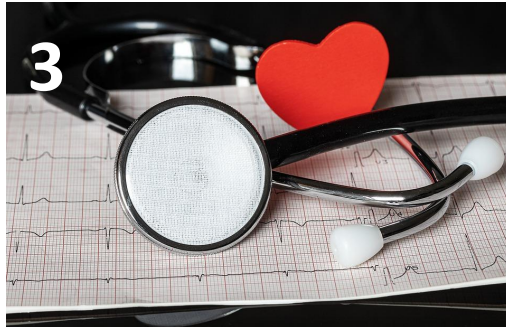
*KIT Institute of **Sports and Sports Research***



2

Chemotion
Electronic Lab
Notebook

*KIT Institute of **Biological and Chemical Systems***



3

AI in
Biomedical
Engineering

*KIT Institute of **Biomedical Engineering***



4

Publication of
Large Datasets

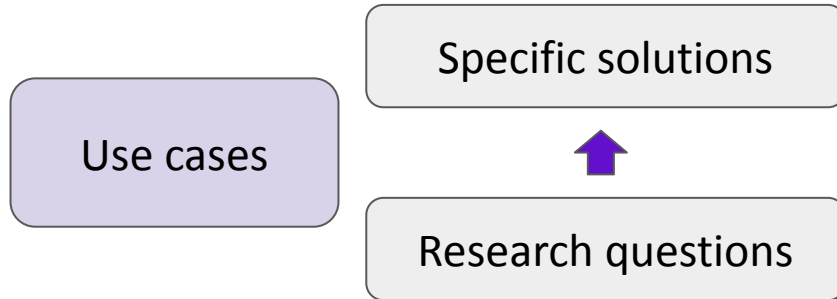
*KIT Institutes of **Meteorology and Climate Research***

From Use Cases to Research Clusters

Use cases

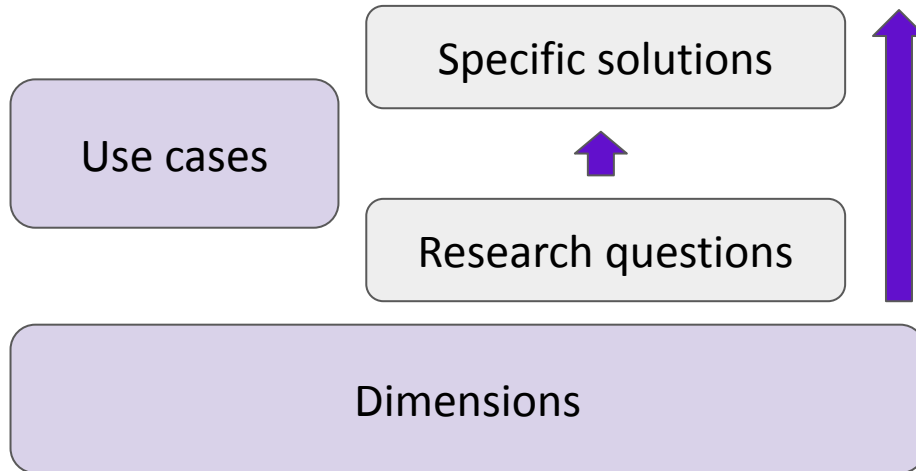
- Impact of digitalisation and AI on science
- Impact of digitalisation and AI on reception of science in society
- Overarching challenges of a technical, legal, and ethical nature

From Use Cases to Research Clusters



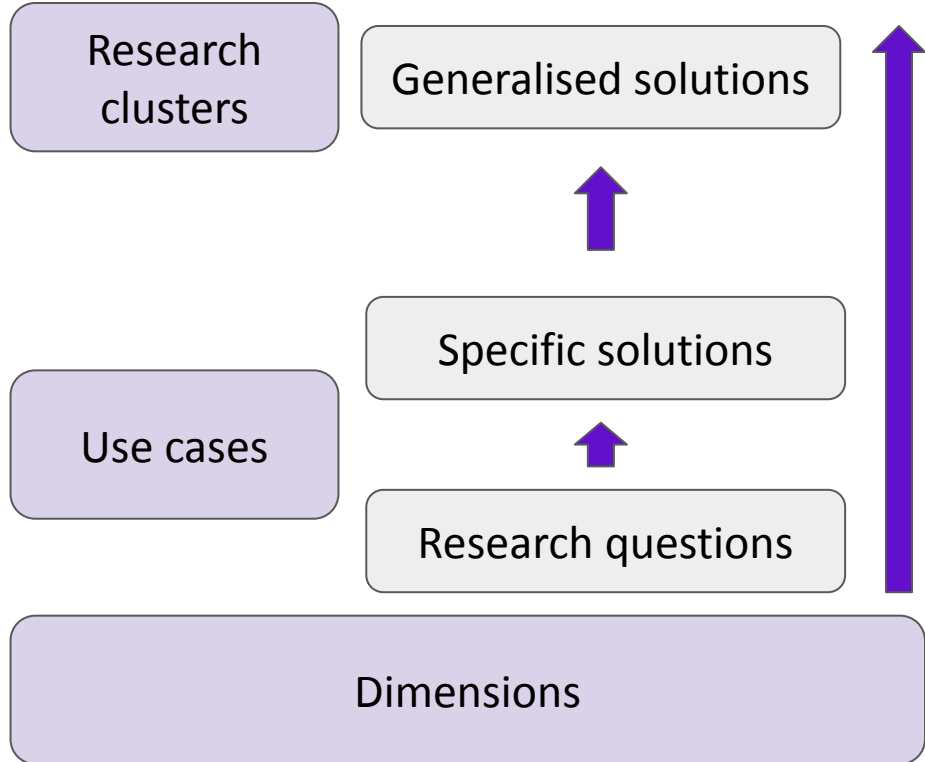
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From Use Cases to Research Clusters



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DiTraRe Dimensions

A. Reflection and Resonance

a dialogue between research and society, interactive process

B. Exploration and Knowledge Organisation

applied AI: represent, organise, and manage domain specific and procedural knowledge

C. Legal and Ethical Challenges

data ethics, data protection, copyright and data law, Task Force “Security”

D. Tools and Processes

digital tools tailored precisely to the needs of researchers



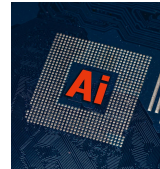
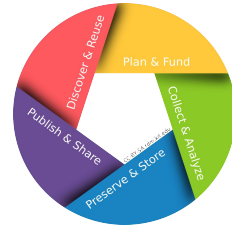
Planned outcomes

- Specific solutions to use cases problems
- Generalised solutions, i.e. best practices, esp. in ethical, legal, security context
- Intensify interactions with society
- Identify new potential threats which come with digitalisation
- Spin-off projects
- Create a networking environment: **collaborate with others!**




Science in the Age of AI: Is Your Research Ready for the Digital Revolution?

- paradigm shift towards **digital** data collection, -management and analysis
- **high quality data** is the basis for good science and ML/AI
- research infrastructures needed for all **stages of the research cycle**
- research **processes are changing** through digitalisation
- **AI** may lead to even more **radical changes** - if we look at the **speed of development**
- How can we **reflect** on the way **how science is conducted** at this speed?
 - ... in all of DiTraRe's **dimensions**, starting with our **use cases**?
 - What are **effects** the **on science system, epistemology, trust** in science by the public?
 - what role plays a **human in the loop** if we can't **scale** our understanding as quickly as AI?



Short history of digitalisation in science

Philosophical Foundations of AI

- 
- **350 BCE - Aristotle:**
 - a. philosophical foundation of AI; introduced “psyche” (soul) and symbolic reasoning, unique to humans
 - b. Developed early theories of perception, reasoning, and consciousness as “actuality”
 - **17th c. Leibniz** asked “what kind of machine is the mind?” and developed logical calculus
 - **20th c.: Wiener, Shannon, Church, Turing, von Neumann** formalised thought via control, information, and computation theories
 - **Mid-20th c.:** Cognitive architectures by **Minsky, Piaget, Simon** establish models of learning and reasoning
 - **Modern AI:** Intelligence seen as computational model-building; evolution as learning algorithm

Short history of digitalisation in science



Leibniz ScienceCampus
Digital Transformation
of Research

1703 **Leibniz** develops the **Logical Machine**, **binary number system**. Publishes *Explication de l'Arithmétique Binaire*

1936 **Alan Turing** publishes "*On Computable Numbers*", introducing the **Turing machine**

1938 - 1977 **Introduction of computers and application in Research**

- 1938-1941 First computers by Konrad Zuse: Z1 (1938, binary mechanical), Z3 (1941, first digital computer).
- 1945 Von Neumann Architecture
- 1975 First Personal Computers: Altair 8800 (1975) Intel's 8080 processor, Apple I (1976), Commodore PET (1977), ...
- 1977 First computational DNA sequencing

1970s-1980s **Networking & the Internet and early internet protocols.**

- 1969 ARPANET goes online, connecting four U.S. universities (UCLA, Stanford, UCSB, University of Utah).
- 1983 Internet (TCP/IP protocol) is standardised.
- 1989 WWW: Tim Berners-Lee launches the **World Wide Web**, revolutionising **information access** (web browsers...)

1990s **Open Science movement** - enhances transparency and accessibility. e.g.: 1991 arXiv.org starts

- 2001 Open Knowledge, platforms like **Wikipedia** democratise knowledge and enable **collaborative** content creation.

2000s **Digitisation of Libraries starts**

- 2002 Internet Archive's Million Book Project starts (still relevant: Websites and data disappear - e.g. now in the US)
- 2004 Google and major libraries begin **digitising books at scale** (Project Gutenberg already started in 1971)

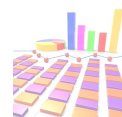
2000-2010s **Data-Driven Research advances**

- 2000 Cloud computing and **Big Data** infrastructures transform data storage and analysis.
- 2008 CERN's Large Hadron Collider produces vast datasets.
- 2009 Jim Gray's **Fourth Paradigm** describes the era of **data-intensive scientific discovery**.
- 2014 Research Tools like **Electronic Lab Notebooks (ELNs)** improve structured data acquisition and reproducibility.

recent years **Artificial Intelligence (AI) & Machine Learning (ML) become central to scientific data analysis**



open science



Today's Symposium Talk by *Sonja Schimmler*



Sonja Schimmler
Fraunhofer FOKUS, Technische
Universität Berlin



Leibniz ScienceCampus
Digital Transformation
of Research

- Prof. Dr. Sonja Schimmler is **Professor for Research Data Infrastructures** at **TU Berlin**, holding the Chair of Research Data Infrastructure.
- **Member** of the **Scientific Advisory Board (SAB)** of the Leibniz ScienceCampus **DiTraRe**.
- Key leadership **roles in NFDI**:
 - Spokesperson of **NFDI4DataScience** (data science & AI infrastructures).
 - Co-Spokesperson of **NFDI4Cat** (catalysis data management).
 - Co-Spokesperson of **Base4NFDI** (core foundational services).
- Research focuses on **digitalisation and openness of scientific workflows**, semantic web, linked data, AI-supported data management, and scalable infrastructures.
- Plays a crucial role in shaping interoperable, trustworthy, and sustainable data infrastructures foundational for AI-driven research across disciplines.

Data Infrastructures as a Foundation for AI Projects

Prof. Dr. Sonja Schimmler

Fraunhofer FOKUS and TU Berlin

Data Infrastructures as a Foundation for AI Projects

Background

About us

Groups

- Fraunhofer: Research Group Lead
- TU Berlin: Guest Professor

Research

- Digitalisation and Opening up of Science
- Research Data Infrastructures

About us

Projects

- Weizenbaum Institute
 - Group Digitalisation and Opening up of Science
- Berlin University Alliance (BUA)
 - Project Berlin Open Science Portal
- National Research Data Infrastructure (NFDI)
 - Consortium NFDI4DataScience
 - Consortium Base4NFDI
- Data Competency Center (DCC)
 - QUADRIGA

Data Infrastructures as a Foundation for AI Projects

Research Focus

Research Focus

Modern research on an internationally competitive level ...

... relies on more and more data

... is no longer possible without digital support

Live Sciences

Natural Sciences

Engineering Sciences

Humanities and Social
Sciences

This leads to a paradigm shift

Research Focus

Scientific progress will only be furthered, if ...

... data becomes available at large scale

... data is linked and machine-interpretable

... specificities of the different disciplines are very carefully taken into account

Live Sciences

Natural Sciences

Engineering Sciences

Humanities and Social
Sciences

This leads to a paradigm shift

Data Infrastructures as a Foundation for AI Projects

Data and Data Infrastructures

Good Scientific Practice

- Increase **transparency and reproducibility** in research

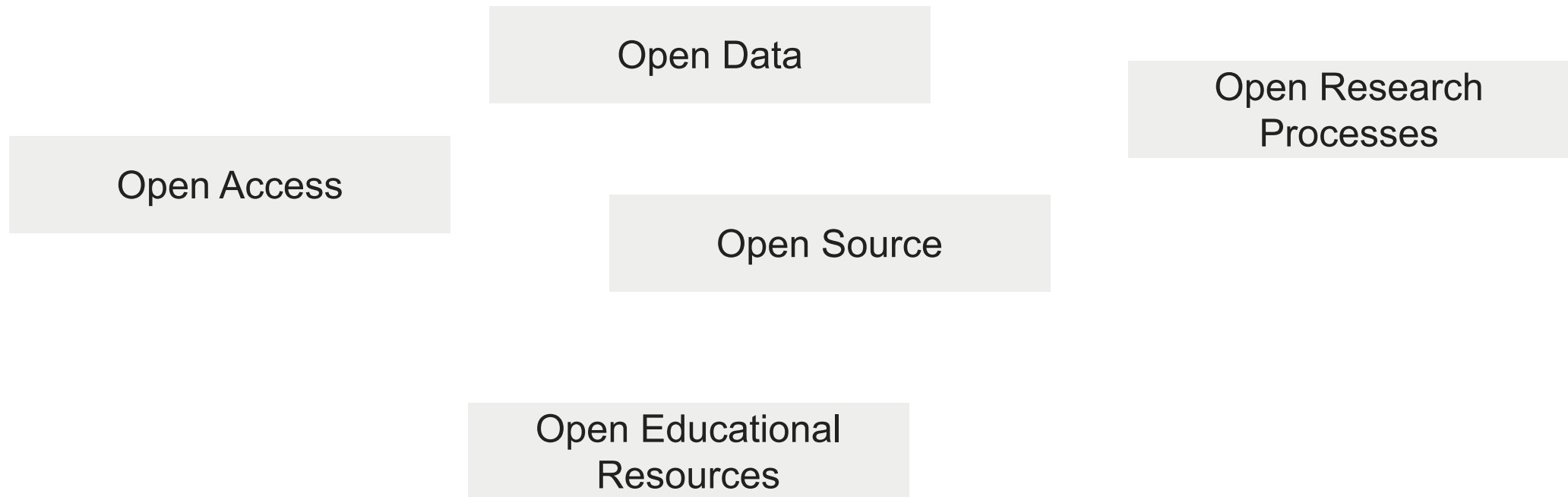


Transparency

Reproducibility

Good Scientific Practice

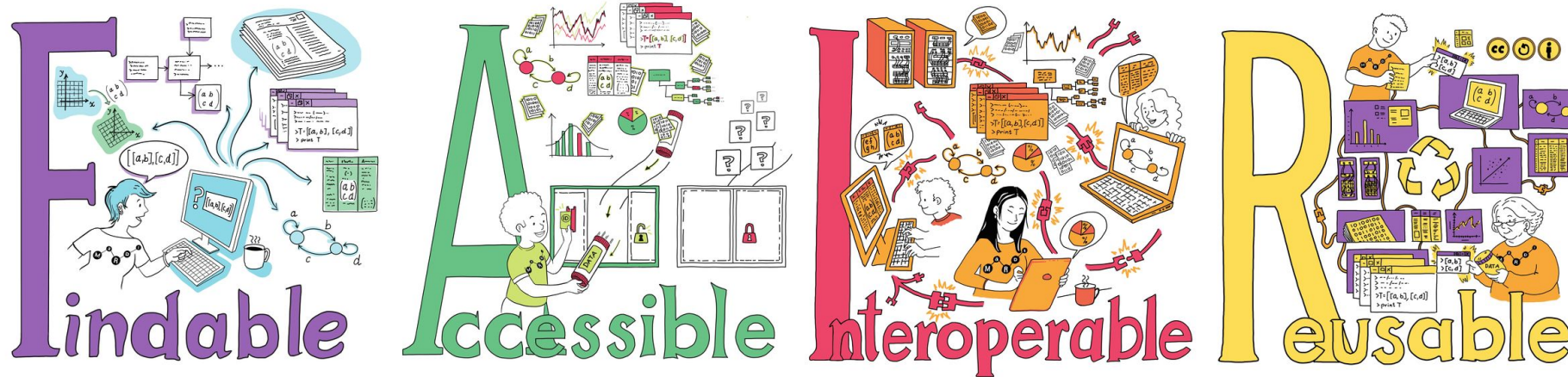
- Foster **open science**



Good Scientific Practice

- Consider **FAIR** principles

(findable, accessible, interoperable, reusable)



by Constanza Rojas-Molina

Good Scientific Practice

- Consider **CARE** principles
(collective benefit, authority to control, responsibility, ethics)



from gida-global.org

Data Infrastructures as a Foundation for AI Projects

AI

Evolution in AI



LLM

- Language model is used in isolation
- Lacks factual knowledge



Retrieval Augmented Generation

- Retrieves unstructured information to augment answers



Knowledge Augmented Generation

- Access to structured information sources, such as databases, knowledge graphs

Evolution in AI



LLM

- Language model is used in isolation
- Lacks factual knowledge



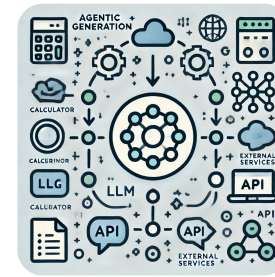
Retrieval Augmented Generation

- Retrieves unstructured information to augment answers



Knowledge Augmented Generation

- Access to structured information sources, such as databases, knowledge graphs



Agentic Generation

- Use of external tools such as reasoners, APIs, computation services



Artificial General Intelligence

- Self-reflection, goal setting

Challenges in AI

**Flood of research
artefacts**

paper, data, models,
scripts/code, ...

**Changing
environment**

data science & AI hype

Challenges in AI

**Flood of research
artefacts**

paper, data, models,
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**Changing
environment**

data science & AI hype

Bias

of training and
evaluation data

**Trustworthiness and
responsibility of AI**

Challenges in AI

**Flood of research
artefacts**

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data science & AI hype

Bias

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**Trustworthiness and
responsibility of AI**

**Good scientific
practice**

transparency &
reproducibility

**Digital scientific
practice**

tools & services

Data Infrastructures meet AI

Generative AI

- Is there a difference in the use of LLMs in the different communities?
- How can we support researchers and the general public that use LLMs?

Data Infrastructures meet AI

Generative AI

- Is there a difference in the use of LLMs in the different communities?
- How can we support researchers and the general public that use LLMs?

Infrastructures and Services for Generative AI

- How to adapt infrastructures to support researchers that use LLMs?

Data Competencies for Generative AI

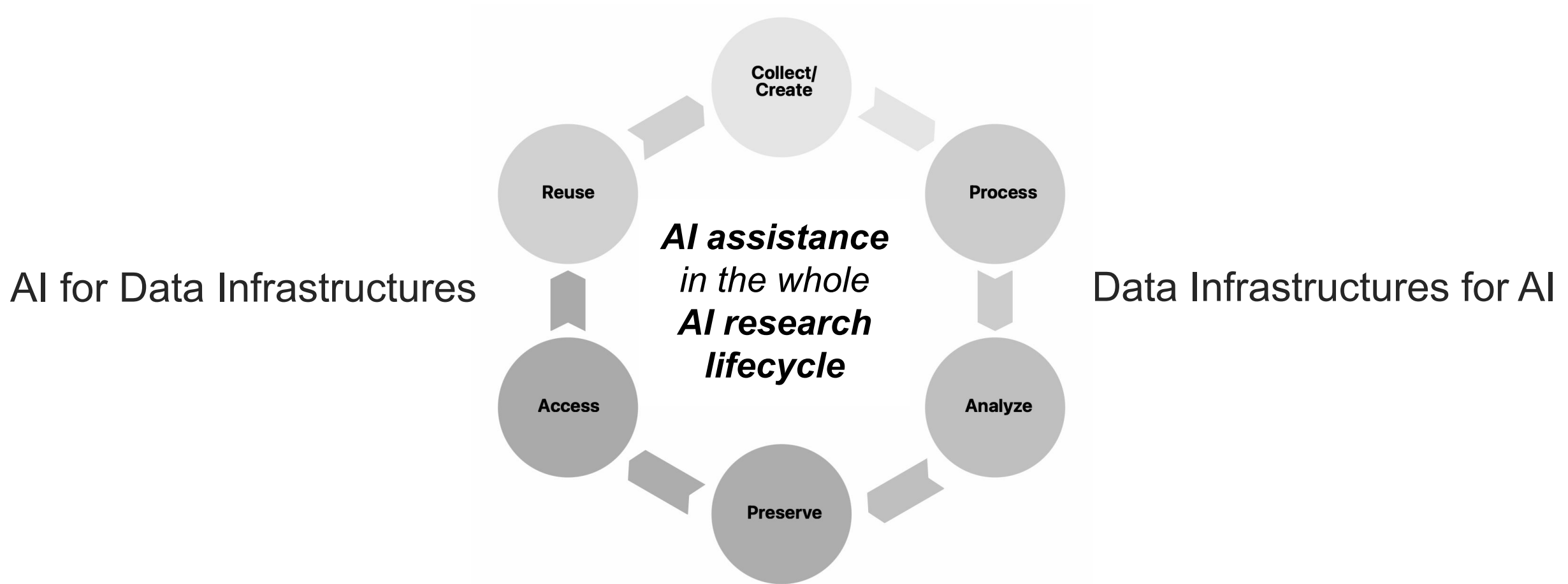
- What new competencies are needed by researchers that use LLMs?

Data Infrastructures meet AI

AI for Data Infrastructures

Data Infrastructures for AI

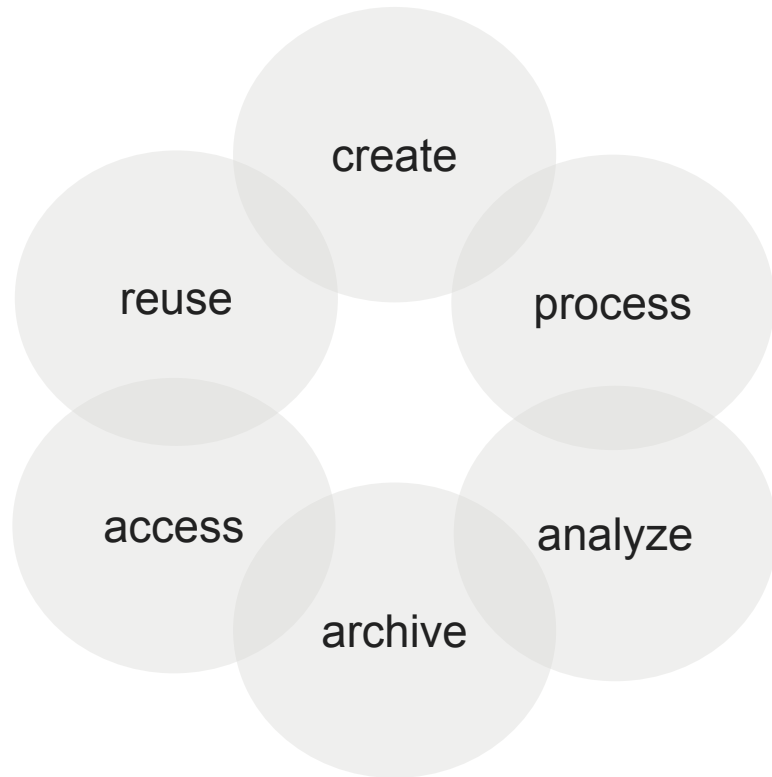
Data Infrastructures meet AI



Data Infrastructures as a Foundation for AI Projects

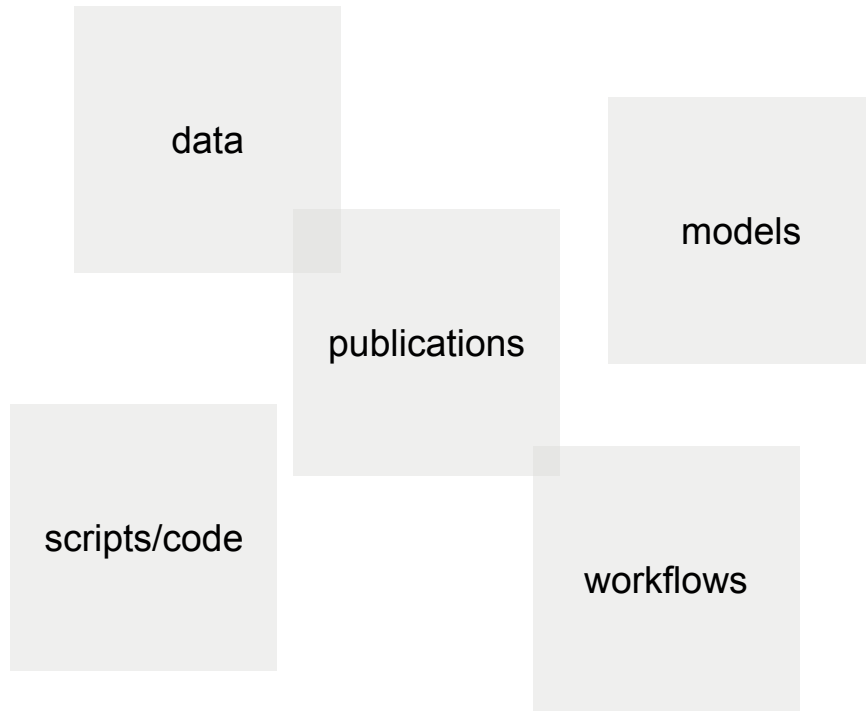
Data Infrastructures

Data Infrastructures



- The whole **research lifecycle** should be considered

Data Infrastructures

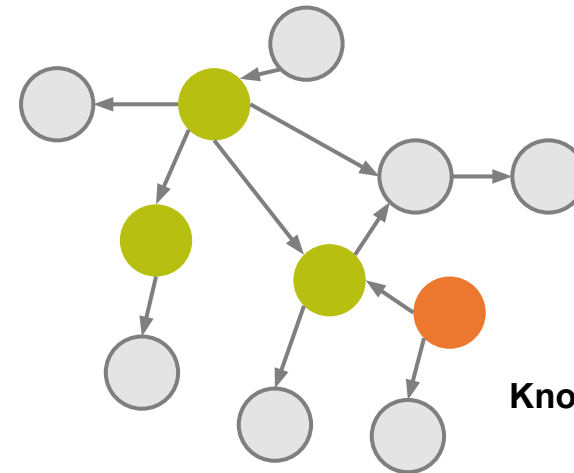
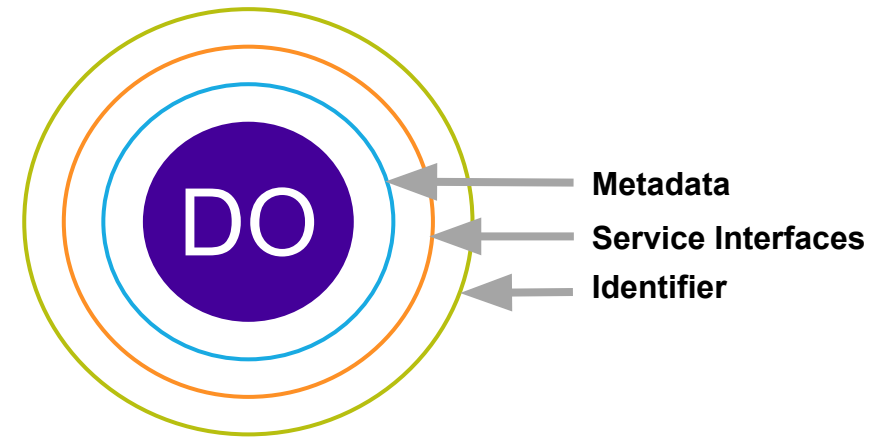


- Publications, data, and other **digital artefacts** (e.g. models, workflows, scripts/code) should be taken into account and should be properly represented

Data Infrastructures

- Digital artifacts should be enriched with **metadata** and should be **linked** for contextualization
- The technical foundation is formed by **(research) knowledge graphs** and **FAIR digital objects**

FAIR Digital Objects (FDOs)



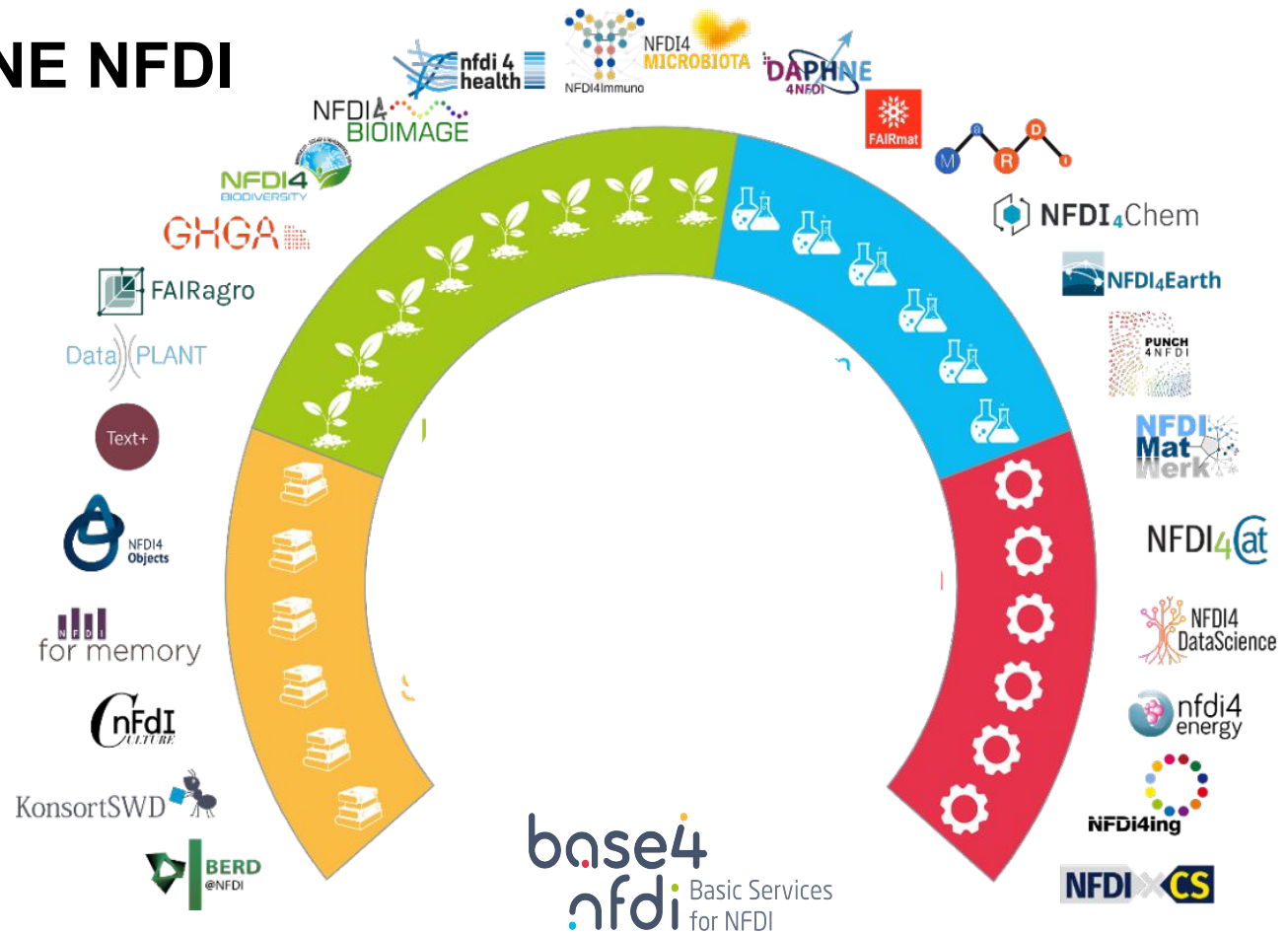
Knowledge Graphs (KGs)

Data Infrastructures as a Foundation for AI Projects

Projects: NFDI and NFDI4DS

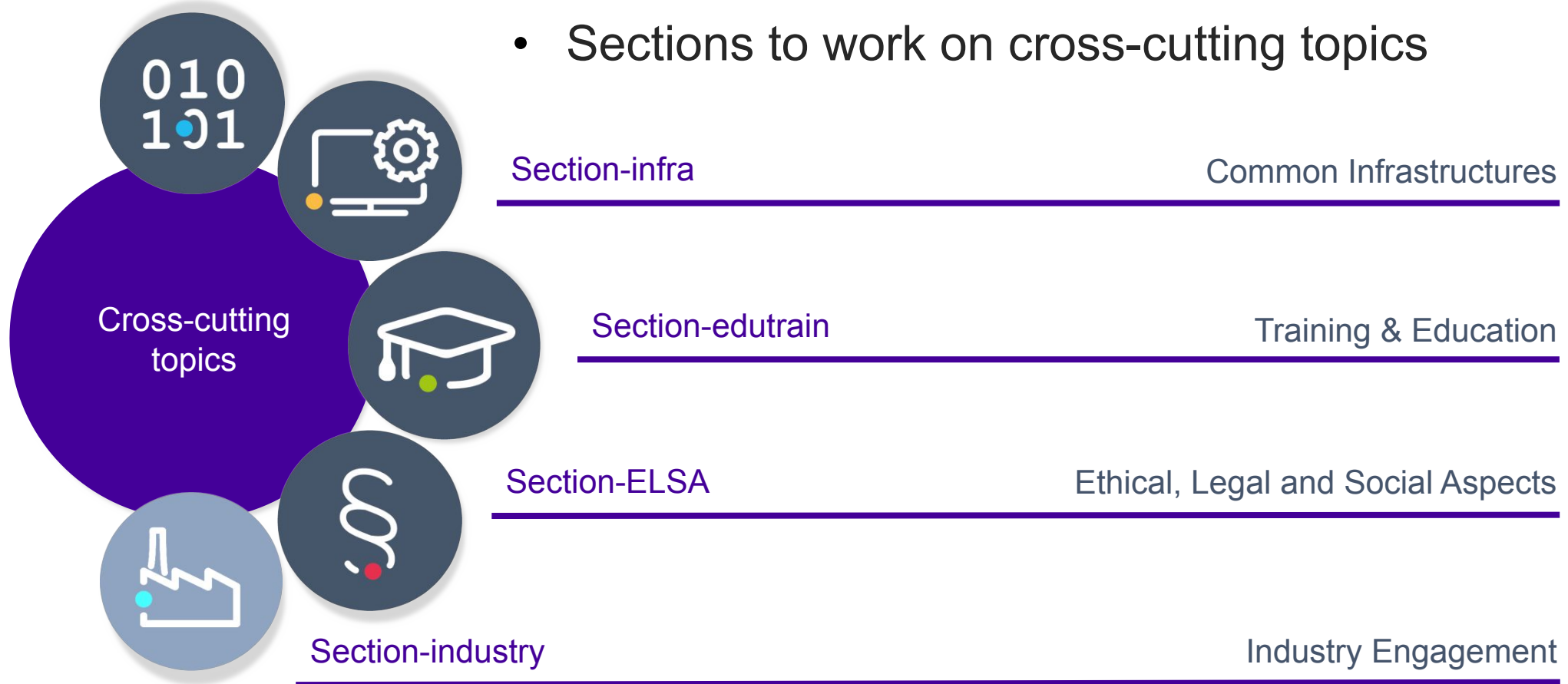
National Research Data Infrastructure (NFDI)

- NFDI to set up a **German National Research Data Infrastructure**
 - The goal is to build **ONE NFDI**
- 26 NFDI consortia



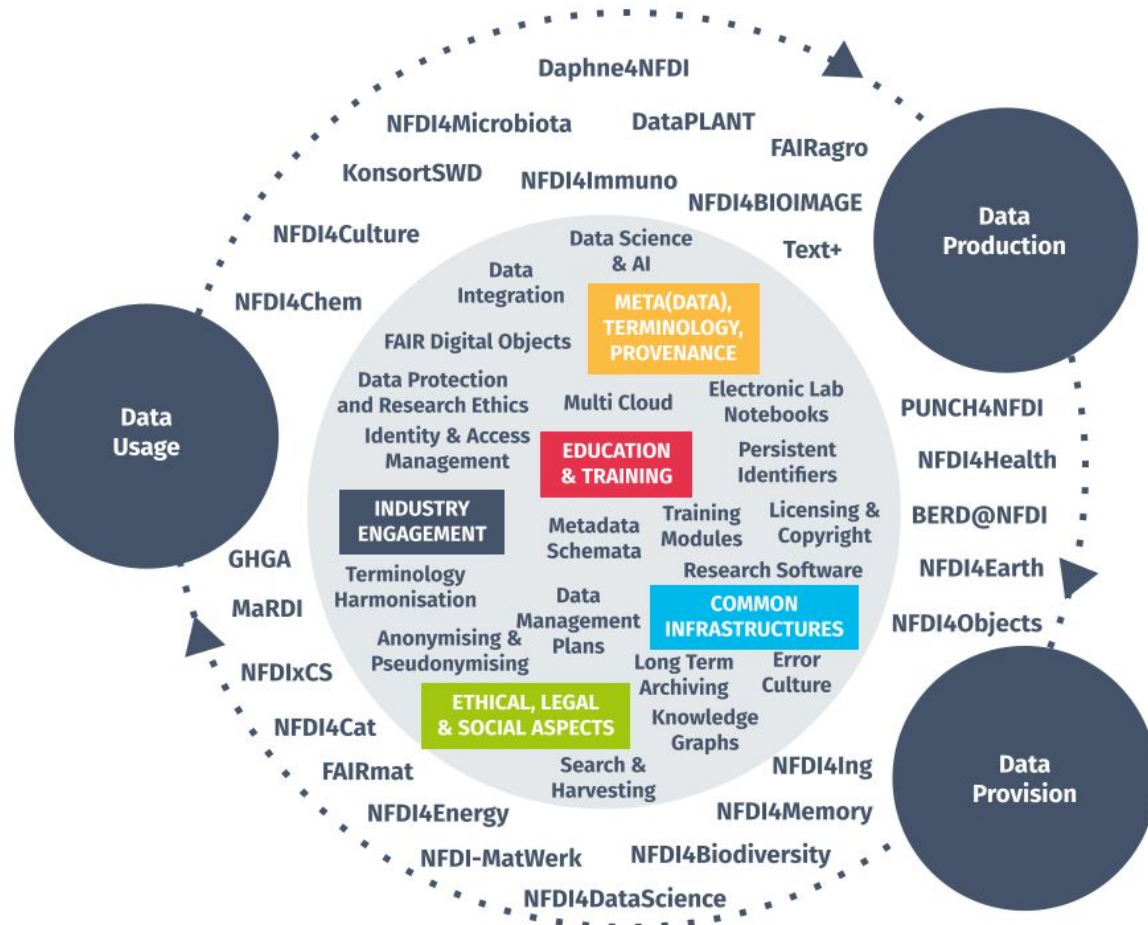
National Research Data Infrastructure (NFDI)

- Sections to work on cross-cutting topics



National Research Data Infrastructure (NFDI)

- Base4NFDI to develop basic services



IAM4NFDI

Identity & Access Management

Supported by: Section Common Infrastructures

PID4NFDI

Persistent Identifier Service

Supported by: Section Common Infrastructures

TS4NFDI

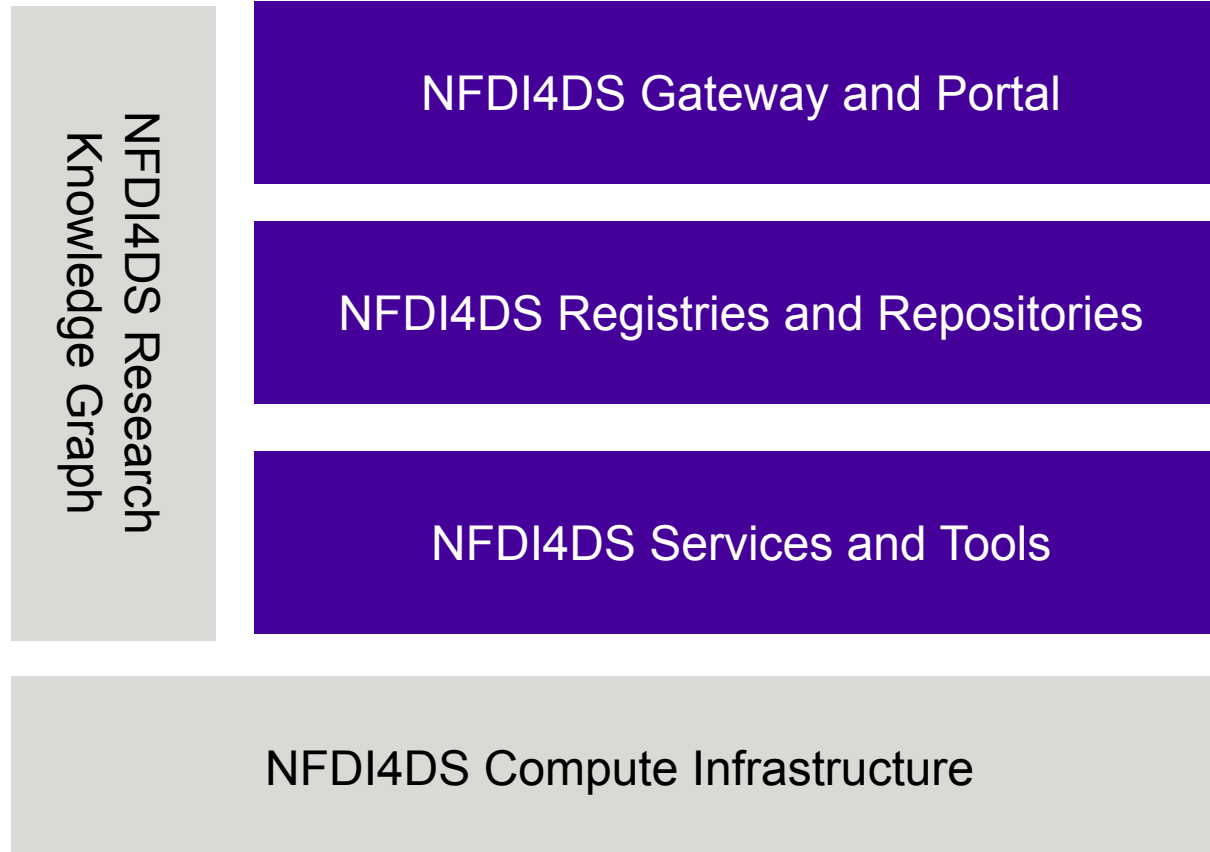
Terminology Services

Supported by: Section Metadata, Terminologies, Provenance

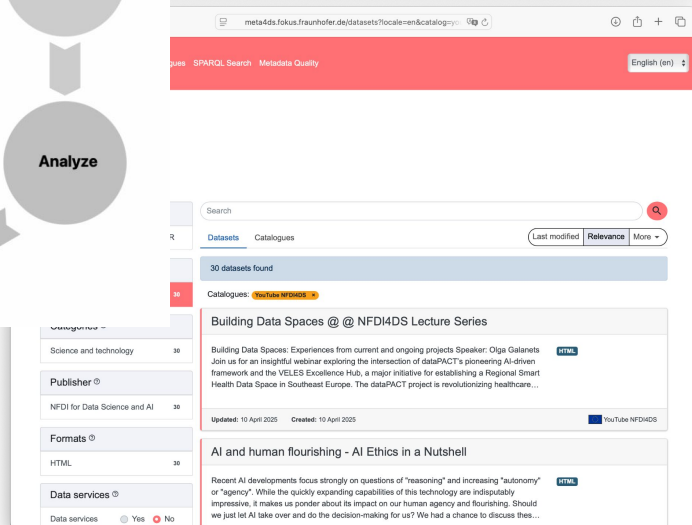
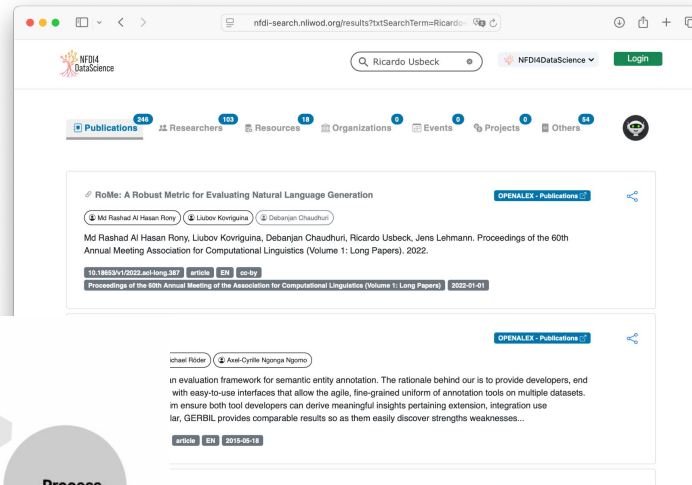
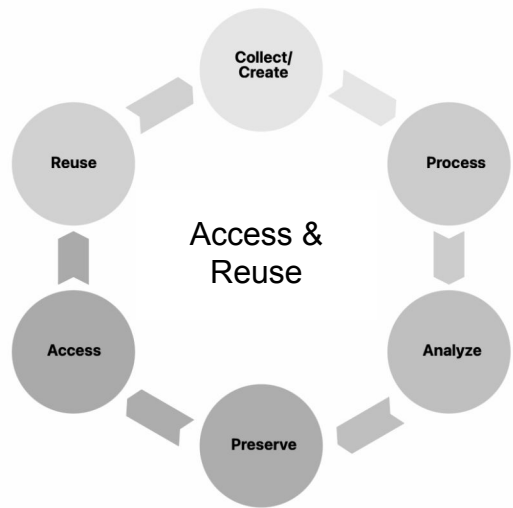
Data Infrastructures as a Foundation for AI Projects

NFDI4DS - Infrastructures

NFDI4DS: Service Portfolio



NFDI4DS: Service Portfolio – Gateway and Portal



NFDI4DS: Service Portfolio – DBLP

dblp
computer science bibliography

search dblp

Sören Auer

> Home > Persons

Person information

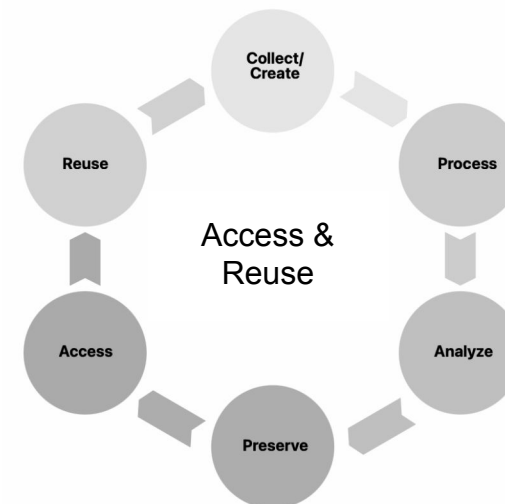
2020 – today

2024

- [j63] Azanzi Jiomekong, Allard Oelen, Sören Auer, Anna-Lena Lorenz, Lars Vogt: **Food information engineering**. *AI Mag.* 45(3): 338-353 (2024)
- [j62] Oliver Karras, Laura Budde, Paulina Merkel, Jörg Hermsdorf, Malte Stonis, Ludger Overmeyer, Bernd-Arno Behrens, Sören Auer: **Organizing Scientific Knowledge from Engineering Sciences Using the Open Research Knowledge Graph: The Tailored Forming Process Chain Use Case**. *Data Sci. J.* 23 (2024)
- [j61] Nour Ramzy, Sören Auer, Hans Ehm, Baptiste Perier: **SENS: Semantic Synthetic Integrated Model for Sustainable Supply Chain Analysis and Benchmarking**. *Enterp. Model. Inf. Syst. Archit. Int. J. Concept. Model.* 19 (2024)
- [j60] Salomon Kabongo, Jennifer D'Souza, Sören Auer: **ORKG-Leaderboards: a systematic workflow for mining leaderboards as a knowledge graph**. *Int. J. Digit. Libr.* 25(1): 41-54 (2024)

SPARQL queries

- run query for this person
- highly cited coauthors
- co-cited other authors



NFDI4DS: Service Portfolio – ORKG and ORKG Ask

The screenshot displays the ORKG Ask web interface. At the top, there's a navigation bar with 'Search', 'My library', and 'ORKG' links, along with a 'Sign in' button. Below this, a search query is entered: 'What data science methods can be used for entity linking?'. A search button is visible. To the left, there are filters for 'Year' and 'Language'. A sidebar on the left mentions 'NFDI4 DataScience' and 'NFDI4DataScience'. The main content area shows an 'Answer (based on top 5 papers)' section, followed by a list of search results. The first result is 'Data linking for the semantic Web' by A. Ferrara, A. Nikolov, and F. Scharffe, dated December 2010. The second result is 'A bibliographic study on entity linking' by Eduardo Habib Bechelane Maia and Marcello Peixoto Bax, dated July. The interface includes a 'Got it' button for a disclaimer about the accuracy of the information.

Search query: What data science methods can be used for entity linking?

Search

The generation of this answer in the area of Data Science is supported by NFDI4DataScience.

Filters

Year

Language

Add filter...

ORKG Ask is brought to you by nfdi Nationale Forschungsdaten Infrastruktur

Answer (based on top 5 papers)

Entity linking, a crucial task in data integration and information extraction, employs various data science methods from statistics [1], database [1], natural language processing (NLP) [2], and graph theory [1]. These techniques enable linking textual mentions in natural language to corresponding entities in a knowledge database, addressing issues such as name variation and entity ambiguity [2]. Techniques include probabilistic methods [4], and open-source frameworks such as Dexter [5] support method development and comparison. However, understanding system performance requires investigation of entity linking dataset properties and their impact [3].

Answer

Insights

TL;DR

Data linking for the semantic Web

A. Ferrara • A. Nikolov • F. Scharffe

December 2010

10.4018/jswis.2011070103

IGI Global

Findings in this paper include techniques with roots in statistics, database, natural language processing and graph theory

Data linking is a crucial aspect of ensuring a Web of data and not just a set of unconnected data is:

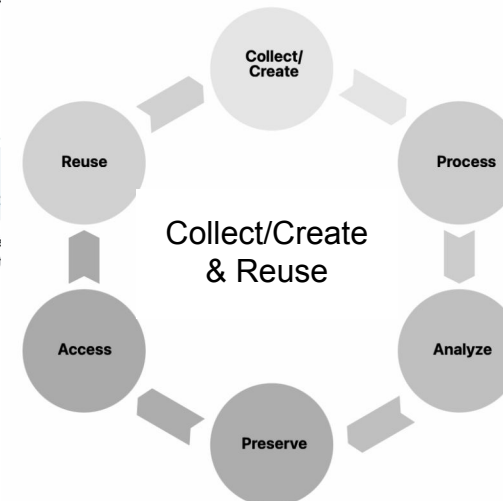
This paper surveys various data linking techniques and tools

A bibliographic study on entity linking

Eduardo Habib Bechelane Maia • Marcello Peixoto Bax

July

LE is a challenging task due like name variation and enti



Data Infrastructures as a Foundation for AI Projects

NFDI4DS - Shared Tasks

NFDI4DS: Shared Tasks

- Development of new tools and services
- Community involvement

SPGQA - Sample : Sheet1			
sample_id	question	questionEntity	answerE
8413	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Arnold S
8414	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Chuck G
8415	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Jeff Flaki
8416	Who was formerly an actor and now a Republican senator?	actor, Republican Party	John McI
8417	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Jon Hunt
8418	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Lindsey I
8419	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Mitch Mc
8420	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Orrin Hat
8421	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Rand Pai
8422	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Rick San
8423	Who was formerly an actor and now a Republican senator?	actor, Republican Party	Roy Blun

KGQA



FoRC & SOMD

- KGQA **@ACL 2024**
 - Knowledge graph question answering
- FoRC & SOMD **@ESWC 2024**
 - Field of research classification for scholarly publications
 - Software mention detection in scholarly publications

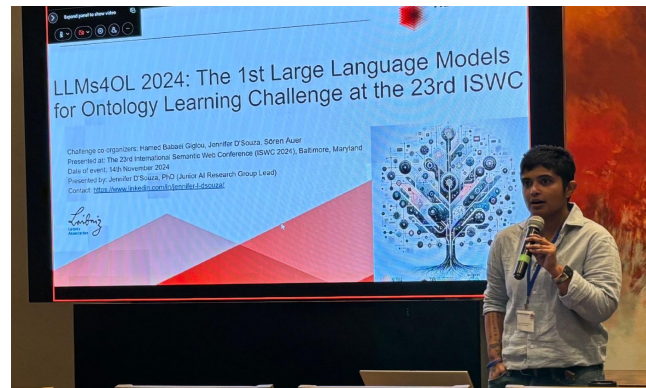
NFDI4DS: Shared Tasks

- Development of new tools and services
- Community involvement

TASK	Dataset	Metric	Score
Template-Based Automatic Search of			
Architectures			
One discovered architecture achieves			
63.2% mean			
IoU on			
CamVid and			
67.8% on			
CityScapes having only 270K parameters			
... .. eval- uation. val			
mIoU, % test			
mIoU, % Params, M Table 2.			
Quantitative results on the test set of CamVid. (†) means that 960x720			
images were used opposed to 480x360. Params, M			
mIoU, % Table 3.			

- (Compact Semantic Segmentation, CamVid, Mean IoU, 63.2)
- (Compact Semantic Segmentation, CityScapes, Mean IoU, 67.8)

SOTA?



LLMs4OL & Scholarly QALD

- SOTA? **@CLEF 2024**
 - State-of-the-art tracking in AI scholarly publications
- LLMs4OL & Scholarly QALD **@ISWC 2024**
 - Large language models for ontology learning
 - Hybrid question answering over scholarly knowledge graphs and text

Data Infrastructures as a Foundation for AI Projects

NFDI4DS - Community Involvement


NFDI4DS: Community Involvement

- **Requirements Elicitation**
 - Surveys, interviews, workshops, classes
- **User Testing**



User Testing @ CoRDI

Cassie



Early PhD Student
Social Sciences

Hi, I am Cassie. I want to find training material on how to deal with data tailored to my needs.

Domain Knowledge: ★★

Technical Skills: ★

Soft Skills: ★★★★★

Ethical/Legal Skills: ★★★★★

Tasks:

- Learning new skills
- Review literature
- Keep up with community news

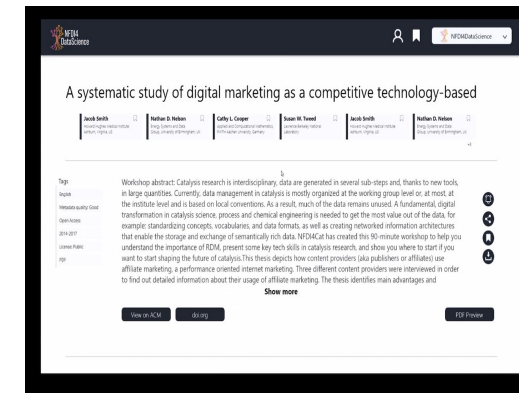
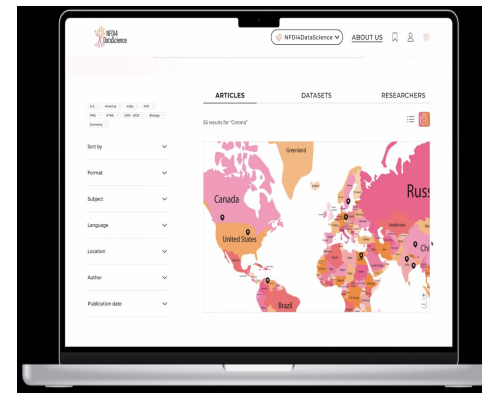
Problems:

- Steep learning curve
- At the same time too much and not enough training material and info

Wishes:

- Training resources tailored to her needs
- Description of typical workflows and processes
- Exchange platform to get in touch with experts

Persona Development @ 4DS Conference



Design of 4DS Access Point @ University Class

NFDI4DS: Community Involvement

- Training and Education



Video Series on Ethical Aspects in AI



Open Science Best Practices



Book on NSLP



Summer School

Data Infrastructures as a Foundation for AI Projects

Summary

Challenges in AI

Flood of research artefacts

paper, data, models,
scripts/code, ...

Changing environment

data science & AI hype

Bias

of training and
evaluation data

Trustworthiness and responsibility of AI

Good scientific practice

transparency &
reproducibility

Digital scientific practice

tools & services

Data Infrastructures meet AI

Generative AI

- Is there a difference in the use of LLMs in the different communities?
- How can we support researchers and the general public that use LLMs?

Infrastructures and Services for Generative AI

- How to adapt infrastructures to support researchers that use LLMs?

Data Competencies for Generative AI

- What new competencies are needed by researchers that use LLMs?

Questions?

Data Infrastructures as a Foundation for AI Projects

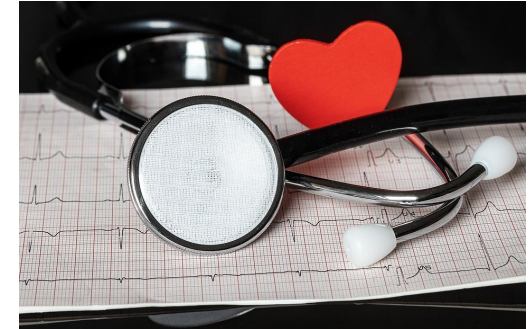
Prof. Dr. Sonja Schimmler
Fraunhofer FOKUS and TU Berlin

Discussion Session

Next Colloquium

- **7 August, 11:00-12:00**
- Join [online](#) or at [KIT Institute of Biomedical Engineering \(IBT\)](#), KIT Campus South
- **Till Keller**, Department of Cardiology and Angiology, Medical Center, University of Freiburg, Bad Krozingen + Justus Liebig University Giessen, Giessen
- Topic: **Use of AI in electrocardiogram (ECG) analysis**
- More info + registration:
www.ditrare.de/en/ditrare-colloquium

DiTraRe use case: [AI in Biomedical Engineering](#)



DiTraRe Symposium

- **2-3 December 2025**
- ZKM Karlsruhe
- Sessions on:
 - Knowledge Representation and AI
 - Law and Ethics in Digitalisation of Research
 - Research Infrastructures
 - Impact on Science and Society
- Call for posters

Website coming soon!



Thank you for joining!

Stay connected

- DiTraRe
 - Website: www.ditrare.de/en
 - Email: ditrare@fiz-karlsruhe.de
 - LinkedIn: www.linkedin.com/company/ditrare
 - Mastodon: social.kit.edu/@DiTraRe
 - YouTube: www.youtube.com/@DiTraRe
 - Zenodo: zenodo.org/communities/ditrare
- Discussion forum: www.ditrare.de/en/forum
- Newsletter: www.ditrare.de/en/newsletter



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